Study Unit 1.2: Conversion and reactor sizing

Fogler (Chapter 2)

SU 1: Fogler, Ch. 1-4, more or less introductory (setting the scene, learning the jargon)

- 1.1 Ch 1: Mole balances
- 1.2 Ch 2: Conversion and Reactor Sizing
- 1.3 Ch 3: Rate Laws
- 1.4 Ch 4: Stoichiometry

SU 2: Fogler, Ch. 5-7, reactor design and analysis; the chemical engineer's bread and butter (still introductory …..)

- 2.1 Ch 5: Isothermal Reactor Design: Conversion
- 2.2 Ch 6: Isothermal Reactor Design: Moles and Molar Flow rates
- 2.3 Ch 7: Collection and Analysis of Rate Data

SU 3 + P: Fogler, Ch. 8 and 11, and Project, somewhat more to practice … (still introductory …..)

- 3.1 Ch 8: Multiple Reactions
- 3.2 Ch 11:Nonisothermal Reactor Design - The Steady State Energy Balance and Adiabatic PFR Applications

1.2. Study Unit 1.2

1.2.1 Conversion

1.2.2 The Levenspiel plot

1.2.3 Reactors in series

1.2.4 Reactors in parallel

1.2.5 The Liquid Hourly Space Velocity (LHSV) and Gas Hourly Space Velocity (GHSV)

1.2.1 Conversion

Conversion (X) is an important parameter in reactor design, and is defined as:

$$X_A = \frac{moles\ of\ A\ reacted}{moles\ of\ A\ fed}$$

Also sometimes termed fractional conversion, it indicates that part of a species that is converted in a reactor

Batch:

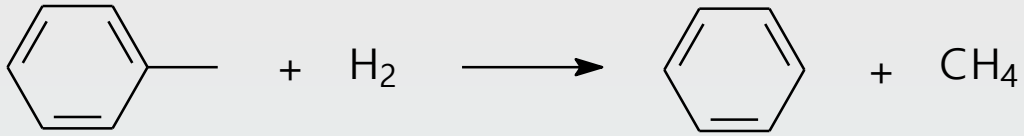
$$X_A = \frac{N_{A0} - N_A}{N_{A0}}$$

[mol]

Continuous:

$$X_A = \frac{F_{A0} - F_A}{F_{A0}}$$

[mol/s]



Consider that 100 kton/yr of toluene is converted in the HDA process, and that on average the process operates 8000 h/yr.

a) Estimate the reactor volume if the average reaction rate of the conversion of toluene equals 1.2 mol/m^3 s *(31 m^3, SU 1.1)*

b) Suggest a shape and dimensions of the reactor *(shape: mostly cylindrical; dimensions: e.g. D = 2.4 m and L = 7.1 m, if aspect ratio = 3; more options possible here)*

c) If toluene is fed to the reactor with 80 mol/s, what is the (single pass) conversion of toluene (X_T)?

1.2.2 The Levenspiel plot

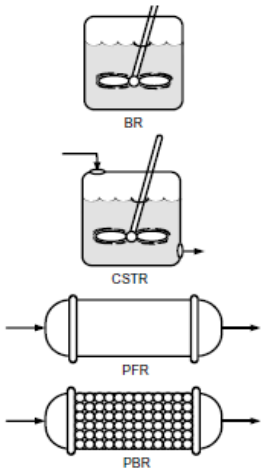


TABLE S1-1 SUMMARY OF REACTOR MOLE BALANCES

Reactor	*Comment*	*Mole Balance Differential Form*	*Algebraic Form*	*Integral Form*
BR	No spatial variations	$\frac{dN_A}{dt} = r_A V$		$t_1 = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V}$
CSTR	No spatial variations, steady state	—	$V = \frac{F_{A0} - F_A}{-r_A}$	—
PFR	Steady state Plug flow	$\frac{dF_A}{dV} = r_A$		$V_1 = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r_A}$
PBR	Steady state Plug flow	$\frac{dF_A}{dW} = r'_A$		$W_1 = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r'_A}$

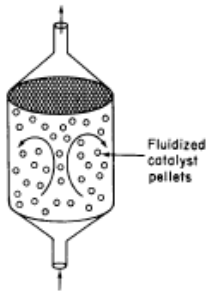
The conversion can be "plugged in" the mole balance equations:

Batch: $$X_A = \frac{N_{A0} - N_A}{N_{A0}}$$

Continuous: $$X_A = \frac{F_{A0} - F_A}{F_{A0}}$$

TABLE S2-1 MOLE BALANCE FOR BR, CSTR, PFR, AND PBR TERMS OF CONVERSION

	Differential Form	*Algebraic Form*	*Integral Form*
Batch	$N_{A0}\frac{dX}{dt} = -r_A V$		$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$
CSTR		$V = \frac{F_{A0}(X_{out} - X_{in})}{(-r_A)_{out}}$	
Fluidized CSTR		$W = \frac{F_{A0}(X_{out} - X_{in})}{(-r'_A)_{out}}$	
PFR	$F_{A0}\frac{dX}{dV} = -r_A$		$V = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r_A}$
PBR	$F_{A0}\frac{dX}{dW} = -r'_A$		$W = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r'_A}$



If we inspect the design equations of the CSTR and the PFR a bit closer

CSTR: $$V = \frac{F_{A0}X}{(-r_A)_{out}} \longrightarrow V = \left(\frac{F_{A0}}{(-r_A)_{out}}\right)X$$

PFR: $$V = F_{A0}\int_0^X \left(\frac{dX}{-r_A}\right) \longrightarrow V = \int_0^X \left(\frac{F_{A0}}{-r_A}\right)dX$$

The ratio **(F_{A0}/-r_A)** is important in sizing reactors, and the reactor volume is inversely proportional to (1/-r_A)

Reaction rate data can only be obtained from experiments, and the following example is on the gas-phase isomerisation reaction **A → B**, carried out at 500 K and 830 kPa, with pure A as initial charge to the reactor

The following experimental data are obtained:

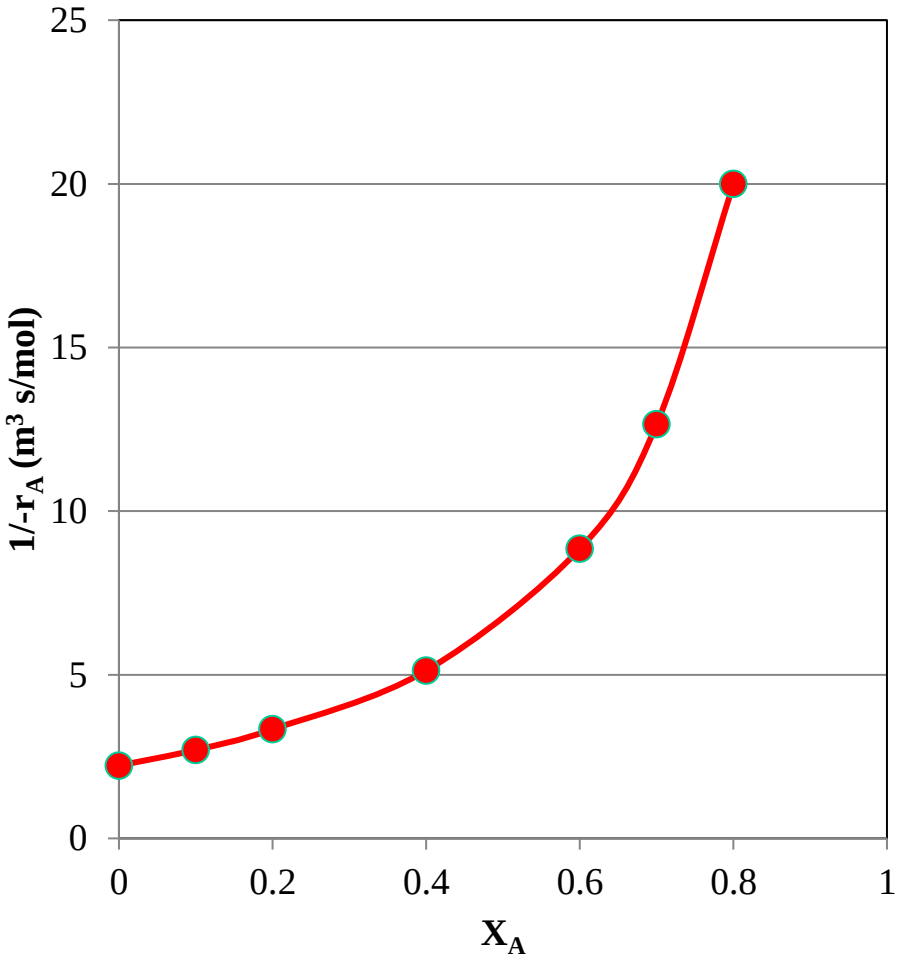
X_A	$-r_A$ (mol/m^3 s)
0	0.45
0.1	0.37
0.2	0.30
0.4	0.195
0.6	0.113
0.7	0.079
0.8	0.05

Can you explain the reaction rate decreasing with conversion?

This is typical for all reactions with an order > 0 (more on this in SU 1.3)

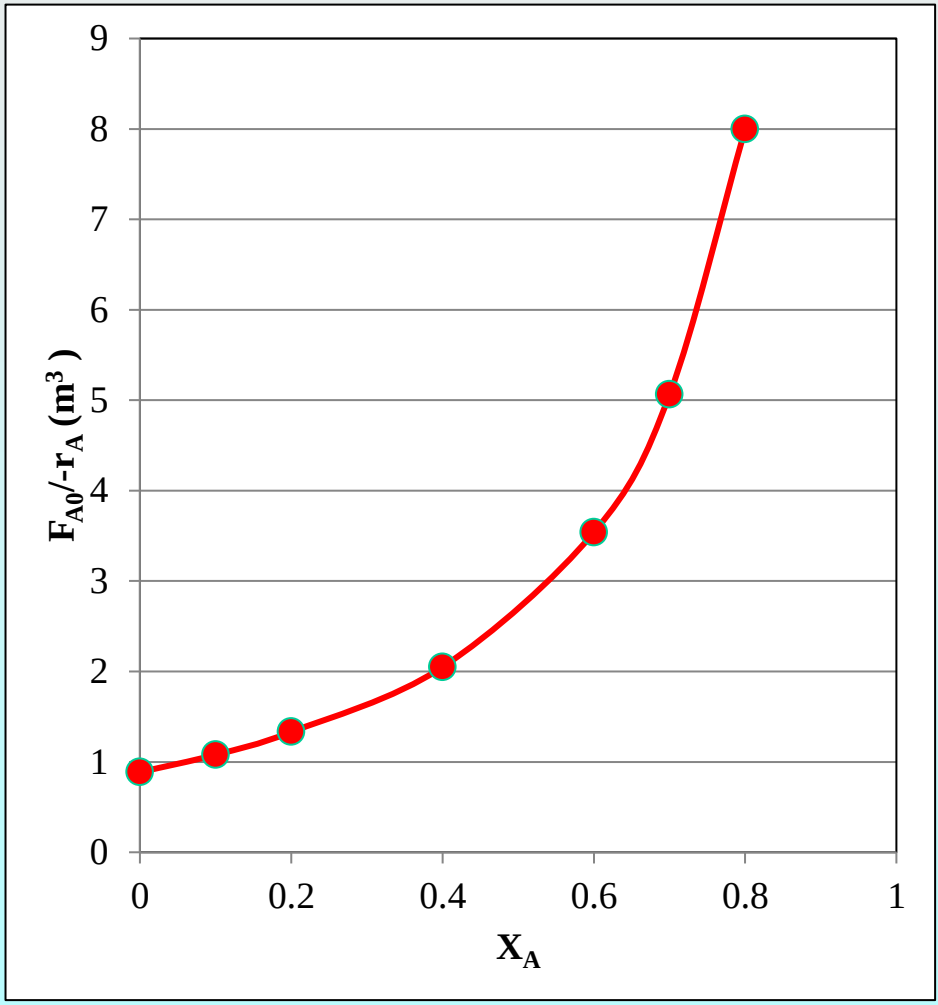
$(1/-r_A)$ as a function of conversion

X_A	$-r_A$ (mol/m^3 s)	$-1/r_A$ (m^3 s/mol)
0	0.45	2.22
0.1	0.37	2.70
0.2	0.30	3.33
0.4	0.195	5.13
0.6	0.113	8.85
0.7	0.079	12.7
0.8	0.05	20.0



If $F_{A0} = 0.4$ mol/s

X_A	$-r_A$ (mol/m^3 s)	$-1/r_A$ (m^3 s/mol)	$-F_{A0}/r_A$ (m^3)
0	0.45	2.22	0.89
0.1	0.37	2.70	1.08
0.2	0.30	3.33	1.33
0.4	0.195	5.13	2.05
0.6	0.113	8.85	3.54
0.7	0.079	12.7	5.06
0.8	0.05	20.0	8.00



Irreversible reaction:

(A → B): V → ∞ as X →1

Reversible reaction (A ↔ B):

V → ∞ as X →X_{eq}

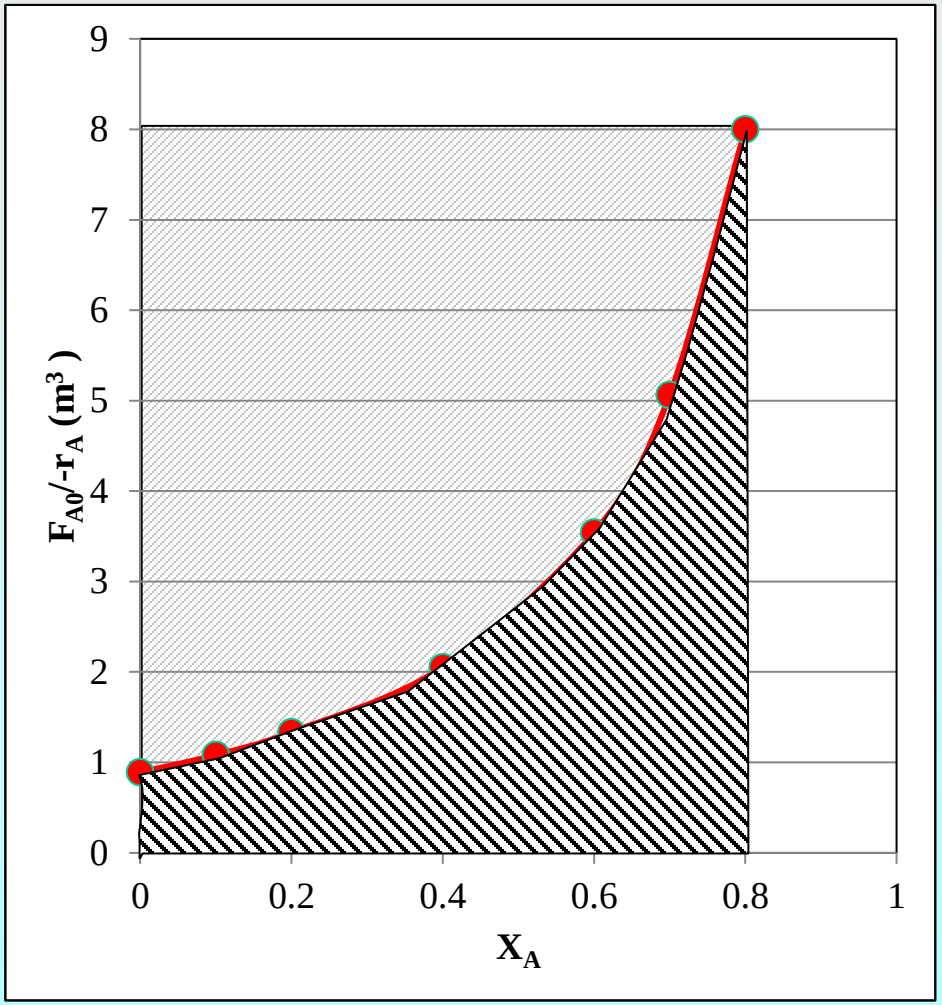
CSTR: $$V = \left(\frac{F_{A0}}{(-r_A)_{out}}\right) X$$

PFR: $$V = \int_0^X \left(\frac{F_{A0}}{-r_A}\right) dX$$

What volume do I need to obtain an 80% conversion (X_A = 0.8)?

$V_{CSTR} = (0.8)*8 = 6.4\ m^3$

$V_{PFR} \sim 2.15\ m^3$



Levenspiel plot

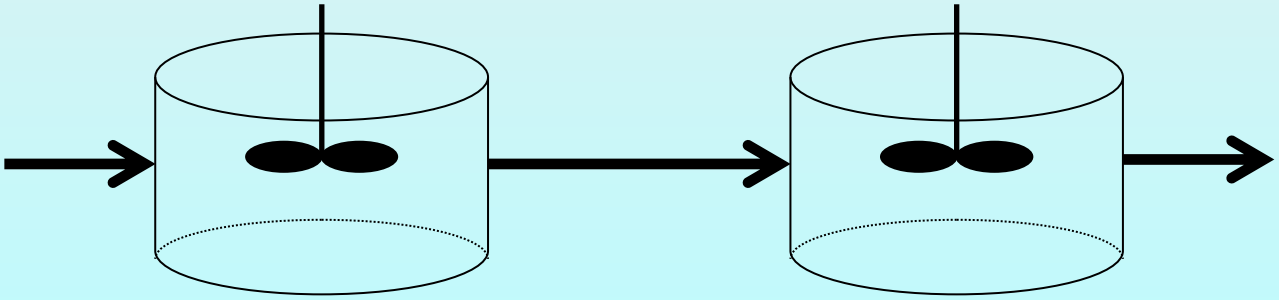
1.2.3 Reactors in series

Reactors in series

Often not only 1 reactor is used, but reactors are used in series or parallel

We start by analysing CSTR's in series

Let's consider two CSTR's in series (again for the irreversible reaction A → B, in which the reaction rate was studied in the previous section), and find again solutions (for V) for 80% conversion.

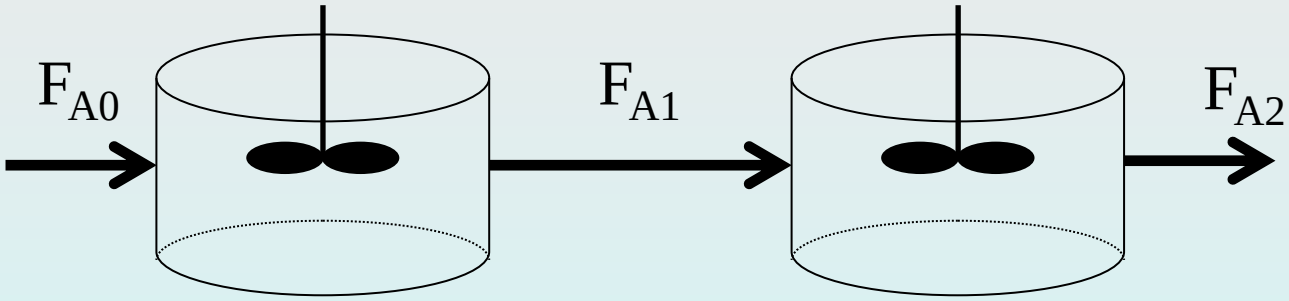


CSTR 1 CSTR 2

Design equation for CSTR:

$$V = \left(\frac{F_{A0}}{(-r_A)_{out}} \right) X$$

Design equation for CSTR: $$V = \left(\frac{F_{A0}}{(-r_A)_{out}}\right) X$$



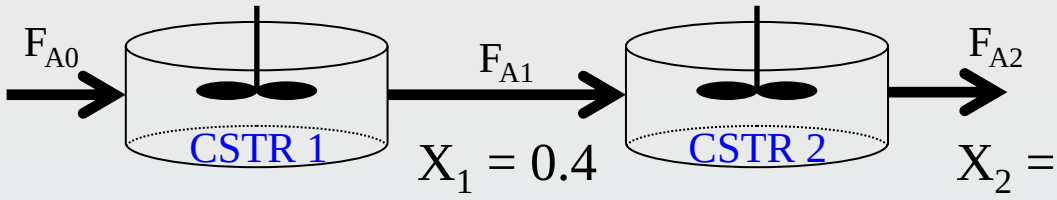
CSTR 1 CSTR 2

$$V_1 = \left(\frac{F_{A0}}{(-r_{A1})_{out}}\right) X_1$$

$$V_2 = \left(\frac{F_{A1}}{(-r_{A2})_{out}}\right) X_2$$

$$V_2 = \left(\frac{F_{A0}}{(-r_{A2})_{out}}\right) (X_2 - X_1)$$

We can *e.g.* design the reactors in such way that the same amount of A is converted in each CSTR.

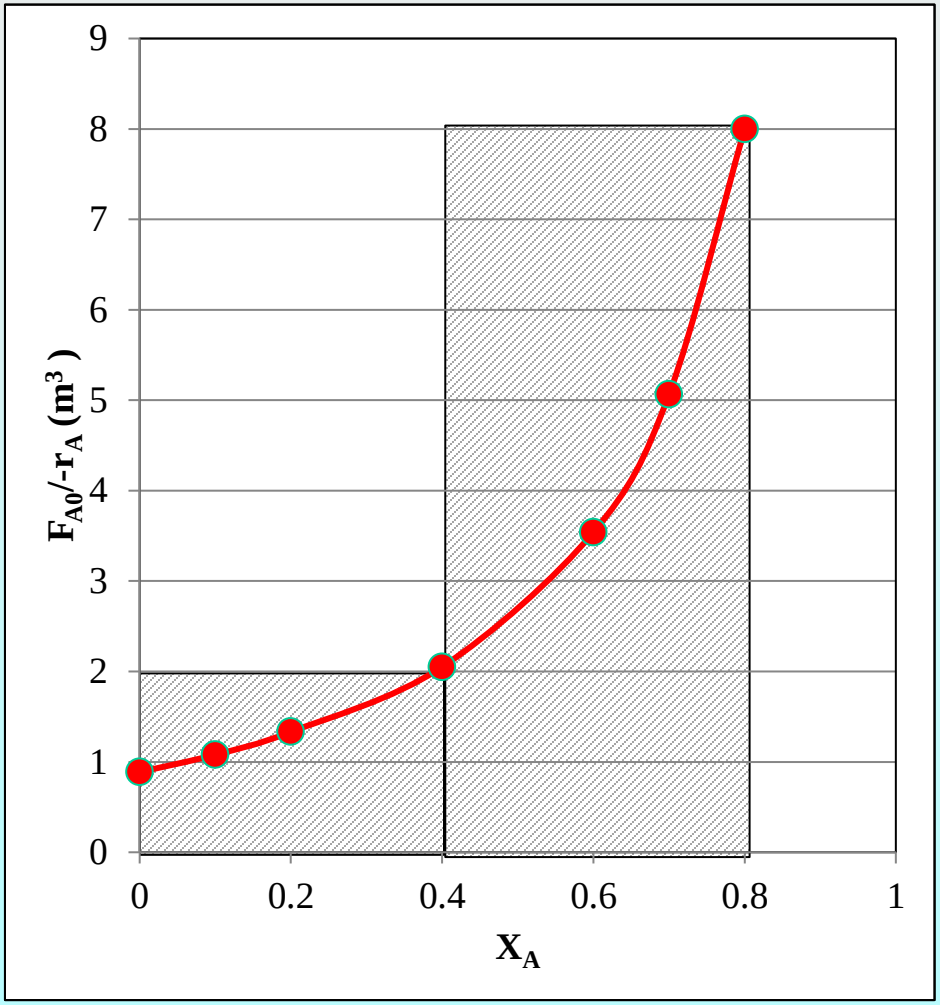


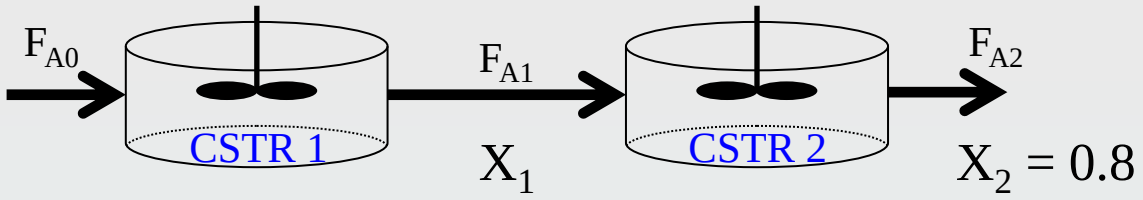
$V_{CSTR1} = (0.4)*2.05 = 0.82\ m^3$

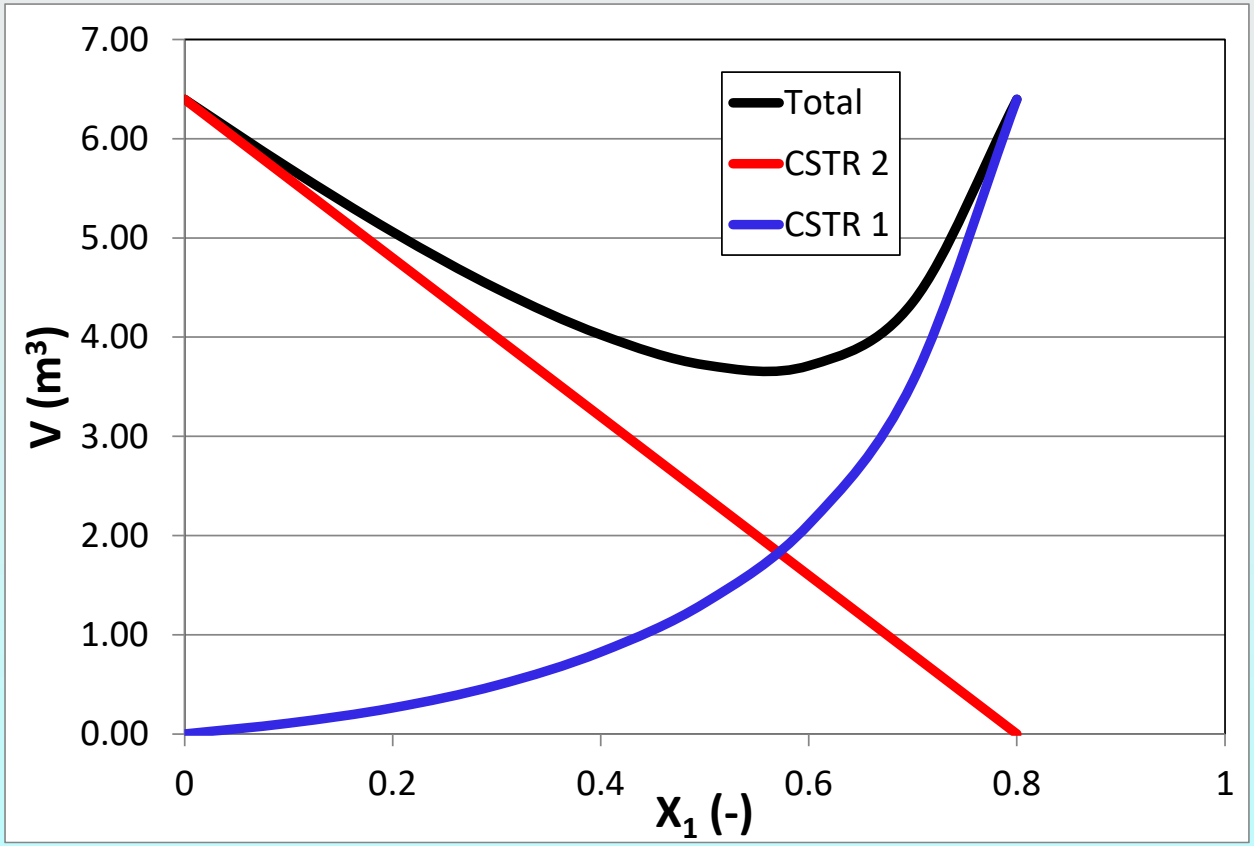
$V_{CSTR2} = (0.4)*8 = 3.2\ m^3$

$V_{total} = 4.02\ m^3$

Compare to the volume of ***6.4 m³*** *if 1 CSTR is used and comment.*







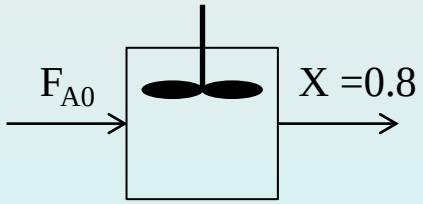
V_{CSTR1}, V_{CSTR2} and V_{TOTAL} as a function of conversion in the CSTR 1 (X_1)

Minimum reactor volume at $V_{CSTR1} = 1.71\ m^3$ ($X_1 = 0.57$), $V_{CSTR2} = 1.96\ m^3$; $V_{total} = 3.67\ m^3$ (compared to $V = 6.4\ m^3$ if 1 CSTR is used)

The total volume of the CSTRs depends on how many CSTRs are used in series

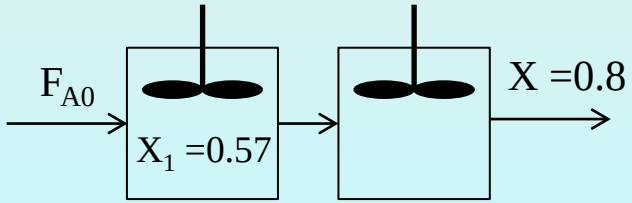
If equally sized CSTRs are used:

N = 1:



$V_{total} = V_{CSTR} =$ **$= 6.4\ m^3$**

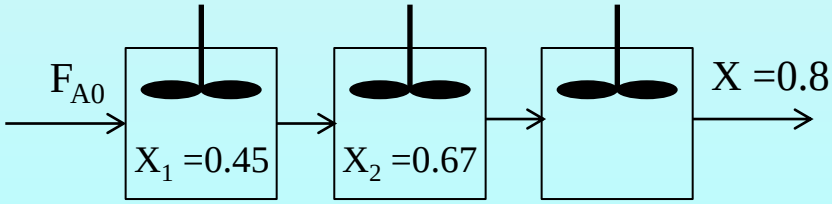
N = 2:



$V_{CSTR} = 1.83\ m^3$

$V_{total} =$ **$3.66\ m^3$**

N = 3:



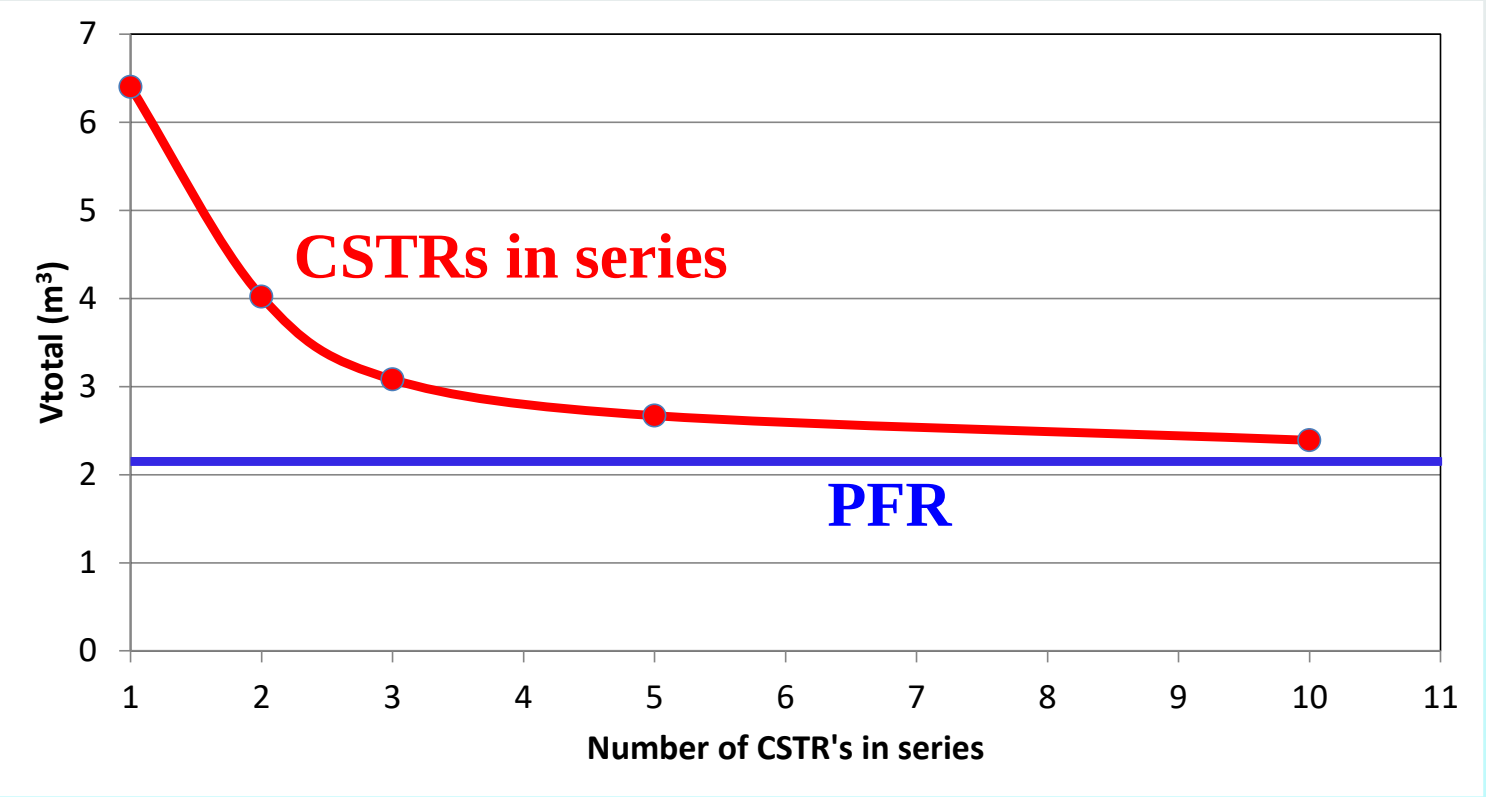
$V_{CSTR} = 1.03\ m^3$

$V_{total} =$ **$3.09\ m^3$**

Exercise: Confirm yourself (by calculation), that for N=3, 3.09 m^3 is needed

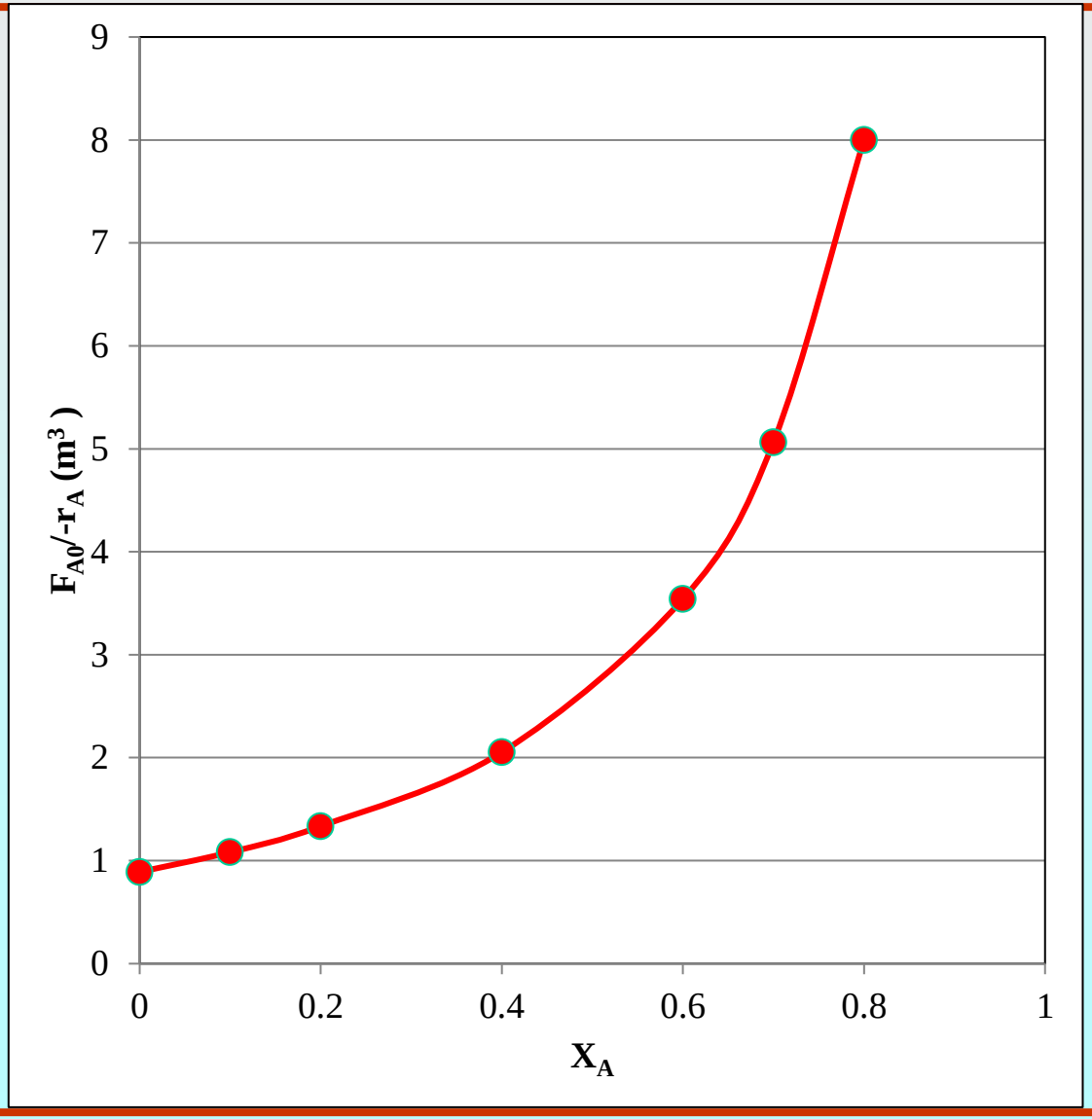
N = 5: $V_{CSTR} = 0.53\ m^3$; $V_{total} =$ **$2.65\ m^3$**

N = 10: $V_{CSTR} = 0.24\ m^3$; $V_{total} =$ **$2.40\ m^3$**



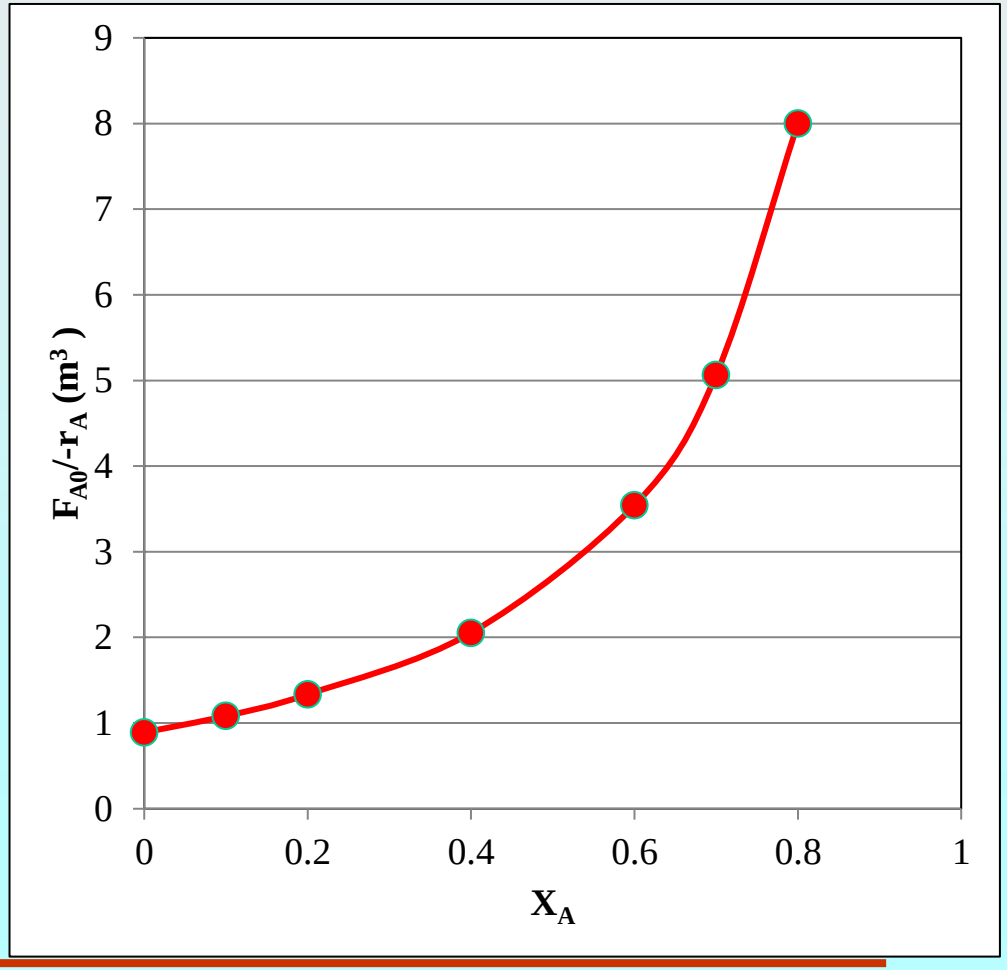
Total CSTR volume as a function of amount of CSTRs in series in comparison to a PFR *(for chemical system as detailed in Example 2.2)*

A PFR can be modelled as infinite CSTRs in series, which can be illustrated using a Levenspiel plot



PFR: $$V = \int_0^X \left(\frac{F_{A0}}{-r_A}\right) dX$$

What do you think of carrying out this reaction in a series of PFR's, in terms of conversion?



Exercise

Consider an exothermic reaction, carried out in an adiabatic reactor:

A → B $\qquad -r_A = k_A(T) \cdot C_A \qquad \Delta h = -$

What happens with the reaction rate if I carry out an exothermic reaction in an adiabatic reactor?

In terms of concentration (w.r.t. conversion)? $\qquad -r_A \downarrow$ if $X \uparrow$

In terms of temperature (w.r.t. conversion)? $\qquad T \uparrow$ if $X \uparrow$ so $-r_A \uparrow$

So in this case, the dependence of the reaction rate with conversion is more complex, and it may well be possible that the reaction rate increases with conversion (so $-1/r_A$ decreases with conversion)

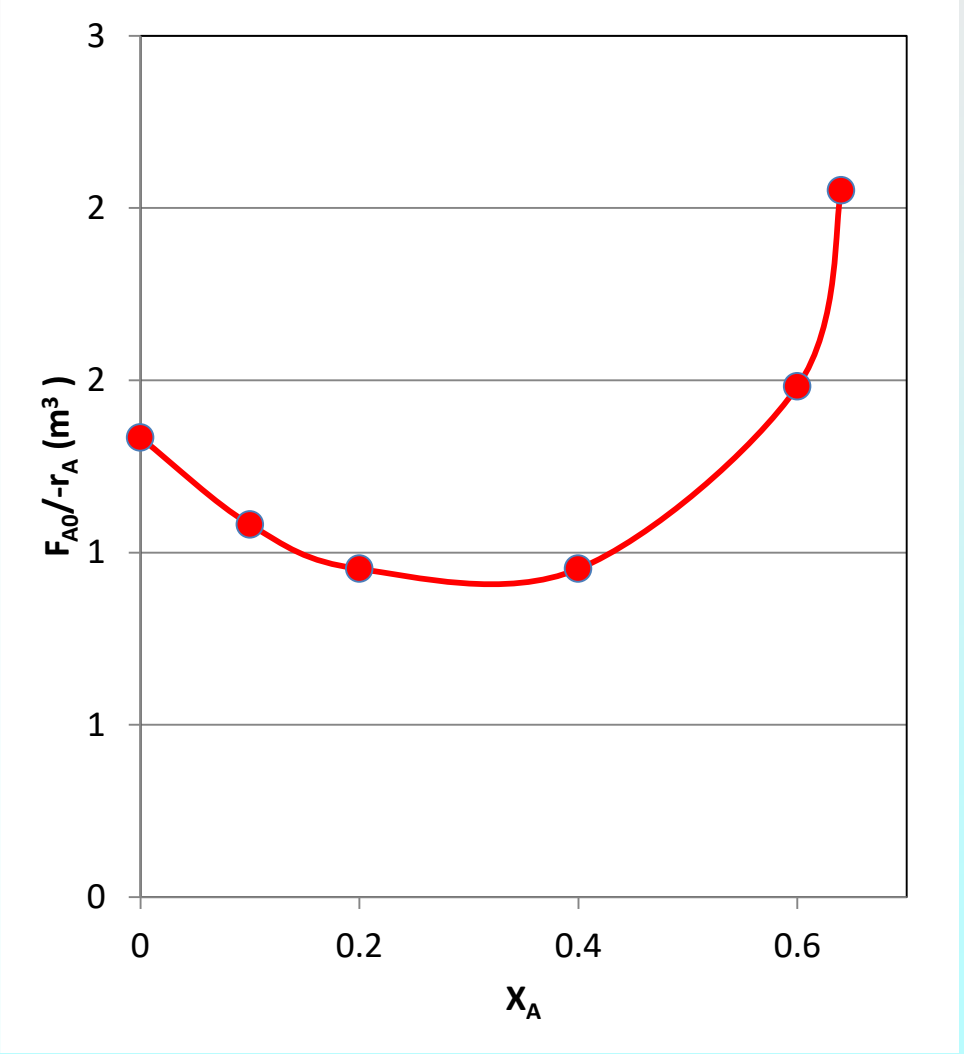
Exercise - continued

If for a certain reaction, the Levenspiel plot has this shape, and 1 reactor will be used, what reactor would you choose

a) If a low conversion is required

b) If a high conversion is required

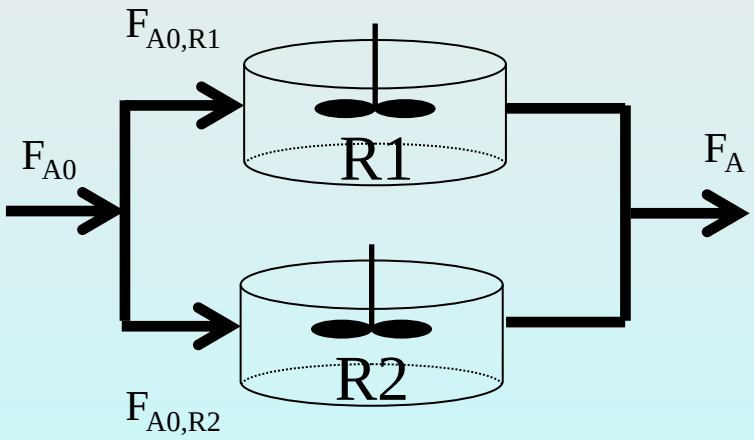
c) If you can choose different reactors, what series of reactors would you choose for optimal (minimal) reactor volume, if a conversion of 60% is required?



1.2.4 Reactors in parallel

$$V = \left(\frac{F_{A0}}{(-r_A)_{out}} \right) X$$

Reactors are sometimes also staged in a parallel configuration



If e.g. $F_{A0,\,R1} = 0.5\,F_{A0}$

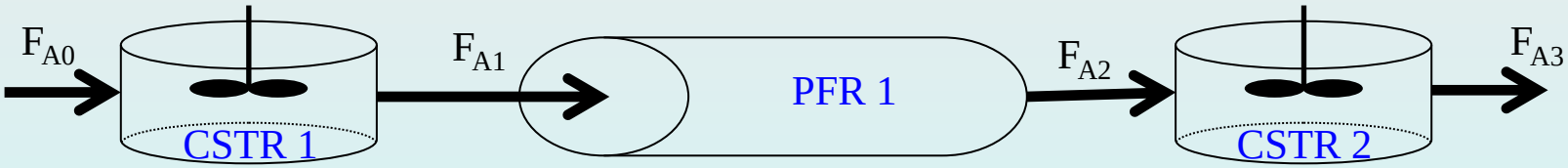
then: $F_{A0,R2} = 0.5\,F_{A0}$

$$\mathbf{F_{A0} = F_{A0,R1} + F_{A0,R2}}$$

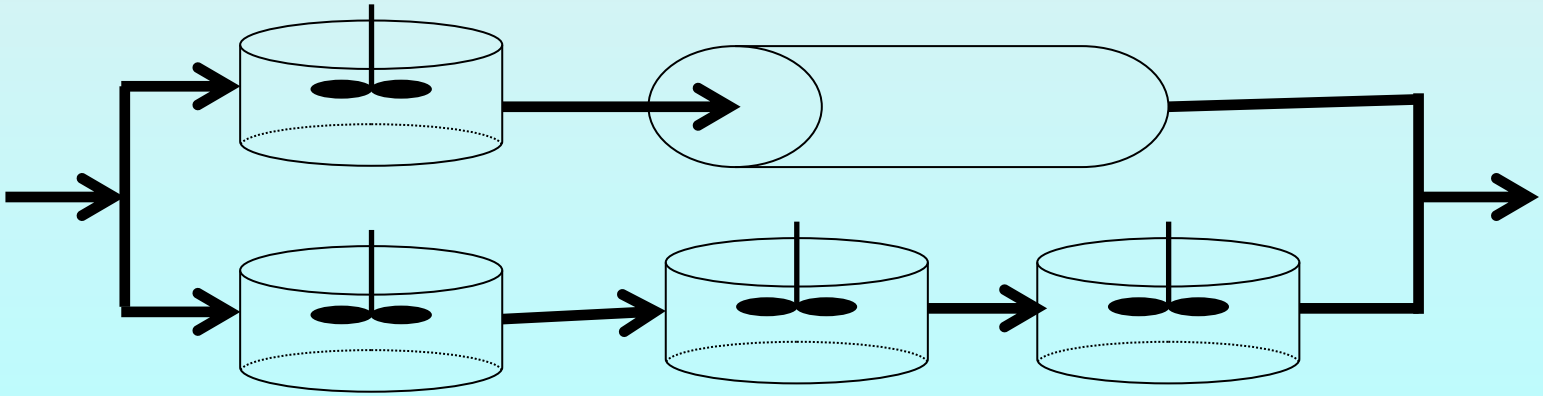
It is then easy to see that $V_{R1} = V_{R2} = 0.5V_0$ (if V_0 is the volume of a single CSTR (with a feed of A of F_{A0}))

Why should one use a parallel configuration, in the chemical process industry?

Configurations with combinations of reactors is also possible



An infinite amount of series/parallel configurations are possible



Sometimes a good configuration of reactors in series can optimise conversion

Practically, it is not always economic to design a reactor / reactor configuration to a specific size

Suppliers only fabricate standard sizes

Sometimes old (already used) reactors are available

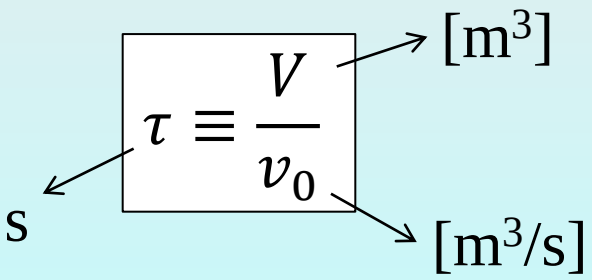
For mechanical and safety reasons, reactors can often not be too large

In Tutorial: Exercise Problem 2-3 for training in the use of series/parallel configuration with given reactor volume!

1.2.5 The Liquid Hourly Space Velocity (LHSV) and Gas Hourly Space Velocity (GHSV)

Some further definitions

The space time, τ, is defined as the ratio of the volume of the reactor (V) and the volumetric flow rate <u>entering</u> the reactor (v_0)



Volumetric flow rates can change during reaction (specifically gas phase reactions); therefore τ is an indication for the residence time of species in the reactor

The Liquid Hourly Space Velocity (LHSV) and Gas Hourly Space Velocity (GHSV), are the reciprocal of the space time, but the volumetric flow rate is often not necessarily measured at the point of entrance of the reactor

$$LHSV = \frac{v_0]_{liquid}}{V}$$

$$GHSV = \frac{v_0]_{gas}}{V}$$

Where the v_0 in the GHSV is often expressed at STP (Nm^3/hr)

As the definition says, the LHSV and GHSV are normally expressed on a per hour basis

Have fast gas phase reactions a high or low GHSV?